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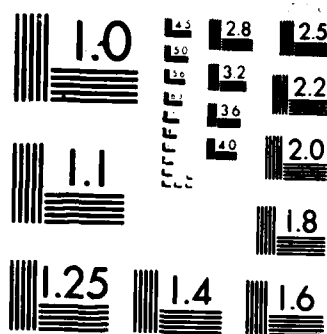
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Numerical Methods for Differential Equations
Final Report

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During the past two years the investigators have been able to develop a computer code which, on the basis of some preliminary experiments, has turned out to be quite competitive with a well established code. The algorithmic development phase of the research has led to several useful results. An eighth order method, which has second, fourth and sixth order methods embedded in it has been developed. The method possesses some of the best features of implicit Runge-Kutta and Gap schemes. A multiderivative generalization of the above schemes has also been realized. A sparse factorization for quasi-Newton type methods has been obtained. Algorithms for solving combined systems of linear and non-linear algebraic equations and matrix splitting have also been developed. A new algorithm has been found for updating the sparse LDU factorization of the approximation to the Jacobian of the system of equations. This method is relatively more efficient than the currently available methods. A practical updating method has been obtained that is in the Broyden family of updates and is in most cases better than the BFGS method. Some effort was directed towards improvement in the stability properties of Boundary Value Runge Kutta (BVRK) methods.

2 Report

$$y'(x) = f(x, y), \quad x \in [a, b]$$
$$q(y(a), y(b)) = 0.$$
$$\hat{y}_i = (1 - \Theta_i)y_0 + \Theta_i y_1 + h \sum_{j=1}^i a_{ij} f(x_0 + c_j h, \hat{y}_j)$$

$$i = 1, \dots, s$$

$$y_1 = y_0 + h \sum_{i=1}^s b_i f(x_0 + c_i h, \hat{y}_j)$$

$$a_{i,j} = 0 \quad \forall j \geq i.$$

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schemes. BVRK methods use information available at both end-points of a subinterval. No information available outside a subinterval is used for approximating the ODE in that subinterval. Because of symmetry, the asymptotic error expansion for the numerical solution has only even powers of mesh-size h . It is possible to develop A-stable BVRK processes, which is desirable. We have developed some techniques which can be used to derive BVRK processes. A quasi-Newton method for the solution of the systems of nonlinear equations arising from the use of these methods, has also been developed. We have derived an eighth order BVRK method which has second, fourth, and sixth embedded in it. We have developed a technique which takes advantage of this natural embedding of methods for generating asymptotically equidistributing grids, and for estimating the error in the numerical solution. We have developed a general purpose adaptive solver based on these ideas. In the future, we hope to make this code compatible with PASVA3 (which is a popular general purpose adaptive code) so that depending on various conditions the final program will either use BVRK processes or Deferred correction.

In [2], we consider a multiderivative generalization of BVRK processes. These methods use fewer derivatives of function f to yield results which are the same as the results for Gap schemes. Hence, these processes will be preferred over Gap schemes if the higher order analytic derivatives are not available.

A general description of sparsity based algorithms that use structural information in handling the model equations is given in [3]. The primary focus is on splitting of equations and variables into two subsets: one large but relatively easy to solve, called the non-basic subset, and the other small but difficult to handle, called the basic subset. The non-basic subset is then solved more often than the difficult basic set. The computer storage is that required by the basic set. Applications in flow networks and energy-economy models are briefly described.

A new quasi-Newton method for sparse matrices arising in various application areas is presented in [4]. In this work sparse triple factorization is used to develop a rank two update.

A class of processes [5] have been found for solving second order boundary value problems of the form $y'' = f(x,y)$, $y(a)=A$, $y(b)=B$. These do not require derivatives of f , and result in nonlinear equations with blocked tridiagonal Jacobians. Specialized techniques have been developed to derive the necessary formulas. The computation of the Jacobians for the discretized systems arising from the use of these formulas is expensive. This makes the ordinary Newton iterations impractical. This paper contains various techniques for approximating and splitting the Jacobians. These techniques are computationally inexpensive and lead to excellent convergence.

An efficient method for handling systems with linear and non-linear subsystems is given in [6]. In this method iterations are needed only for the solution of non-linear subsystems.

Cubic and quintic splines have been utilized in some of the methods for solving differential equations developed by the investigators and others in the past. One of the crucial steps in these techniques involves the solution of band systems. A very efficient general purpose scheme for handling such band systems [7] has been developed. This scheme is also very useful for block banded systems arising in a variety of applications.

A method of order eight that uses cubic splines on quintic splines for solving differential

equations is described in [8].

The Principal Investigator has given invited papers based on some of the research resulting from this grant at two international conferences [9,10]. In [11], we consider the numerical solution of parabolic partial differential equations of Schrodinger type. Most conventional explicit finite difference methods are unconditionally unstable for these problems. Use of explicit Runge-Kutta methods with method of lines also yields unstable results. However, use of an implicit method requires solution of complex systems of algebraic equations. Since, very little is known about large complex systems as compared to real systems, explicit schemes would be preferred over implicit schemes. Also, most explicit schemes can easily be vectorized. In [11], we consider the use of dissipative terms for deriving conditionally stable explicit single step schemes. We also consider use of a pair of methods in an alternating fashion for getting more accurate results. Most of the methods considered in this paper can easily be extended for more general Schrodinger equations.

In [12], we consider the following singularly perturbed two-point boundary value

$$\begin{aligned} -\epsilon u'' + a(x) u' &= f(x, u) \\ u(0) &= g_0, \quad u(1) = g_1. \end{aligned}$$

We assume that a and f are sufficiently smooth functions and that $a(x) \geq \bar{a} > 0$ on $[0, 1]$. Then using the usual splitting one can prove that for ϵ sufficiently small, the solution of the above problem can be represented as

$$u(x; \epsilon) = A(x; \epsilon) + B(x; \epsilon) \exp\left[\frac{1}{\epsilon} \int_x^1 a\right]$$

where A and B , and their derivatives up to an integer K can be bounded on $[0, 1]$ independently of ϵ . For subintervals $[x_{i-1}, x_i]$ and $[x_i, x_{i+1}]$, we consider finite difference schemes of the following form:

$$\begin{aligned} \hat{U}_j &= \theta_j U_{i-1} + \delta_j U_i + \mu_j U_{i+1} - \sum_{k=1}^J \gamma_{jk} f(\psi_k, \hat{U}_k), \quad j = 1, \dots, J \\ \alpha_{-1} U_{i-1} + \alpha_0 U_i + \alpha_1 U_{i+1} &= \sum_{j=1}^J \beta_j f(\psi_j, \hat{U}_j) \end{aligned}$$

where coefficients θ_j , δ_j , μ_j , γ_{jk} , β_j , α_{-1} , α_0 , and α_1 are chosen so that the scheme is exact on a class of functions

$$1, x, \dots, x^n, \exp\left(\frac{1}{\epsilon} \int^x a\right), \dots, x^L \exp\left(\frac{1}{\epsilon} \int^x a\right).$$

First, second and third order methods of this type have been tried on some test problems and they exhibit the same uniform order of convergence as predicted by the theory.

In [13], we consider linear complementarity problems having special structures. A large number of free-boundary problems can be formulated as linear-complementary problems having the properties discussed in this paper.

In [14], a new definition of stability that characterizes the behavior of BVRK methods is being developed.

3 Publications

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